Important Equations from Chapter 2

$$\chi_A = \frac{c_{A\circ} - c_A}{c_{A\circ}}$$

$$c_A = c_{A\circ}(1 - \chi_A)$$

0th Order Irreversible

$$c_A = c_{A\circ} - kt$$

$$\chi_A = kt / c_{A\circ}$$

valid only when t < ($c_{A\circ}/k$)

1st Order Irreversible

A → B

$$c_A = c_{A\circ} e^{-kt}$$

$$c_B = c_{B\circ} + c_{A\circ}(1 - e^{-kt})$$

$$\chi_A = 1 - e^{-kt}$$

2nd Order Irreversible – Uni

A + A → B

$$c_A = \frac{c_{A\circ}}{c_{A\circ} kt + 1}$$

$$c_B = c_{B\circ} + \frac{c_{A\circ}^2 kt}{2(c_{A\circ} kt + 1)}$$

$$\chi_A = \frac{c_{A\circ} kt}{1 + c_{A\circ} kt}$$

2nd Order Irreversible – Bi – Stoich = 1

A + B → C

$$c_A = \frac{c_{A\circ} - c_{B\circ}}{1 - \gamma e^{qt}}$$

$$\chi_A = \frac{\gamma(e^{qt} - 1)}{\gamma e^{qt} - 1}$$

where q = ($c_{B\circ}$ - $c_{A\circ}$)k and $\gamma = c_{B\circ}/c_{A\circ} \neq 1$

2nd Order Irreversible – Bi – Stoich ≠ 1

αA + βB → C

$$c_A = \frac{c_{A\circ}(\beta c_{A\circ} - \alpha c_{B\circ})}{\beta c_{A\circ} - \alpha c_{B\circ} e^{qt}}$$

$$\chi_A = \frac{\gamma(e^{qt} - 1)}{\gamma e^{qt} - 1}$$

where q = [$c_{B\circ}$ – (β/α)$c_{A\circ}$]k and $\gamma = \alpha c_{B\circ}/\beta c_{A\circ} \neq 1$

Autocatalytic

A + B → 2B

$$c_A = \frac{c_{A\circ} + c_{B\circ}}{1 + \gamma e^{qt}}$$

$$\chi_A = \frac{\gamma(e^{qt} - 1)}{1 + \gamma e^{qt}}$$

where q = ($c_{B\circ}$ + $c_{A\circ}$)k and $\gamma = c_{B\circ}/c_{A\circ}$

1st Order Reversible

A ↔ B

$$K_{eq} = \frac{k_1}{k_{-1}} = \frac{c_{B\,eq}}{c_{A\,eq}}$$

$$\chi_{Aeq} = \frac{(K_{eq} - \gamma)}{(K_{eq} + 1)}$$

$$K_{eq} = \frac{(\gamma + \chi_{Aeq})}{(1 - \chi_{Aeq})}$$

$$\chi_A = \chi_{Aeq}(1 - e^{-qt})$$

where $q = \frac{k_1(\gamma + 1)}{(\gamma + \chi_{Aeq})}$ and $\gamma = c_{B\circ}/c_{A\circ}$

Series First Order Irreversible Reactions

A → B → C

$$c_A = c_{A\circ} e^{-k_1 t}$$

$$c_B = \frac{k_1 c_{A\circ}}{k_2 - k_1}\left(e^{-k_1 t} - e^{-k_2 t}\right) + c_{B\circ} e^{-k_2 t}$$

$$c_C = c_{C\circ} + \frac{c_{A\circ}}{k_2 - k_1}\left(k_1 e^{-k_2 t} - k_2 e^{-k_1 t}\right) - \frac{c_{B\circ}}{k_2} e^{-k_2 t}$$

$$t_{\max} = \frac{\ln k_1 - \ln k_2}{k_1 - k_2}$$

Enzyme Kinetics

S + E ↔ ES → P + E

$$-\frac{dc_S}{dt} = \frac{V_{\text{MAX}} c_S}{K_M + c_S}$$

$$V_{\text{MAX}} t = c_{S\circ} - c_S + K_M \ln\left(\frac{c_{S\circ}}{c_S}\right)$$

where $V_{MAX} = k_2 c_{E\circ}$ and $K_M = (k_{-1} + k_2)/k_1$